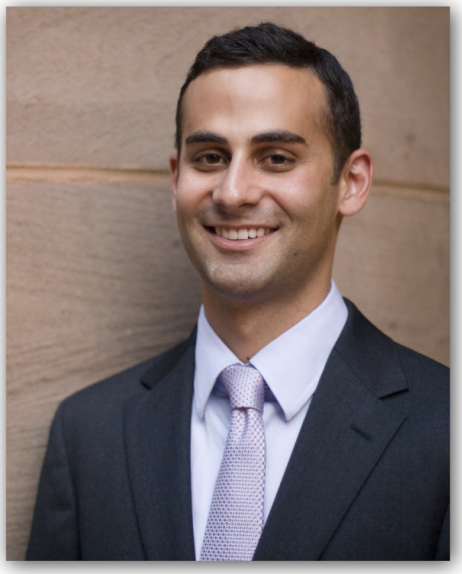
MRSEC SEMINAR SERIES

"Rational Materials Discovery: 'Bottom-up' design of emergent ferroelectricity"



There are two main routes to accelerate materials discoveries for advanced electronic and sustainable energy technologies: serendipitous realization through conventional synthesis or computationally guided growth of novel materials through, *e.g.*, artificial structuring of bulk compounds at the atomic scale. Recently, the launch of the Materials Genome Initiative (MGI) at the national level has reinvigorated the search for new routes to accelerate the discovery of advanced materials for rapid deployment—the aim being to evolve a "hunter and gatherer" discovery paradigm into the cultivation of materials by design.

Within this setting, and motivated by prospects of integrating ferroelectric perovskite oxides into electronic devices to reduce consumer power consumption, I describe in this talk the design methodology and theoretical discovery of a new class of "rotation-induced" ferroelectric materials. Bottom-up engineering of the atomic framework structure, specifically rotations of transition metal octahedra at the unit cell level, is applied to realize ferroelectricity in artificial ABO_3-structured composites formed by interleaving two bulk materials with no tendency to such behavior. This emergent, chemistry-independent, form of ferroelectricity – *octahedral rotation-induced ferroelectricity* – offers a reliable means to externally address and achieve deterministic electric-field control over magnetism. I discuss the required crystal-chemistry criteria, which are obtained using a combination of electronic-structure computations and applied group theoretical methods, to select the compositions and stoichiometries for experimental synthesis. I propose a number of gallate, aluminate, stannate and zirconate compounds that are computationally found to be comparable to the best known ferroelectric oxides and are now under experimental study. I conclude by describing how these findings will contribute to our understanding of not only new forms of ferroic (or anti-ferroic) behavior, but also that this general approach of physical properties by atomistic structure design within the MGI is immediately amenable to other material functionalities.

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